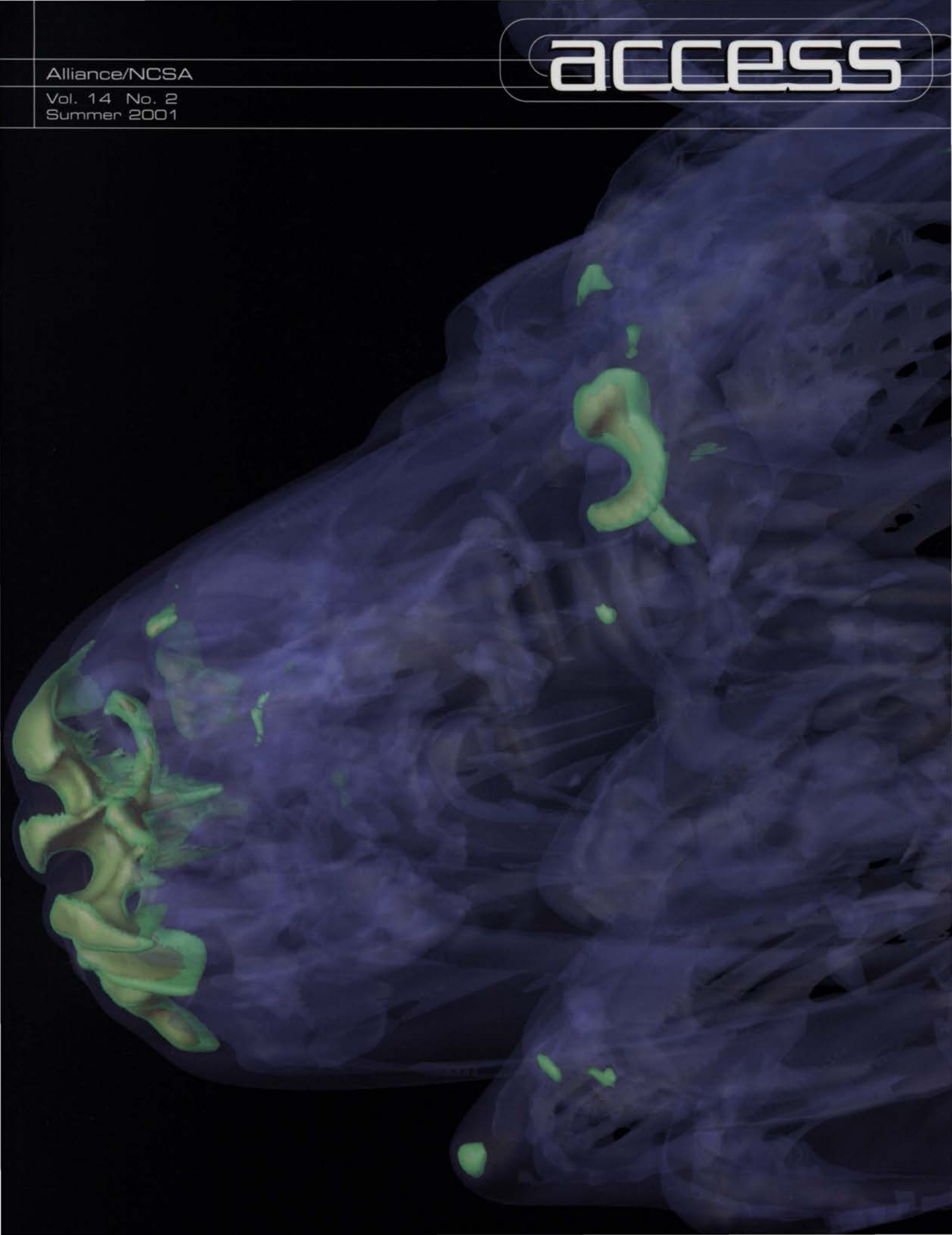


Alliance/NCSA

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# access





NCSA

## access

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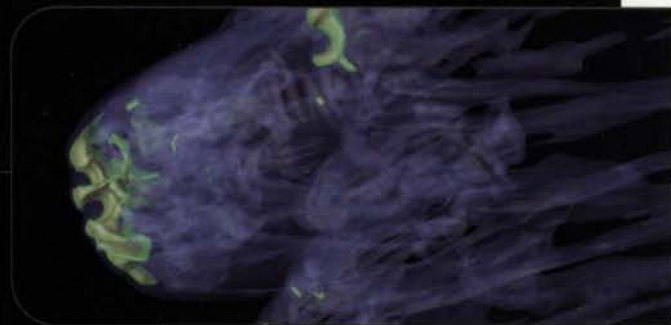
### Who we are

The National Computational Science Alliance (Alliance) is a partnership among more than 50 academic, government, and industrial organizations from across the United States to prototype an advanced computational infrastructure for the 21st century. This model infrastructure, called the Grid, will link together advanced supercomputers, visualization environments, and mass storage devices into a powerful, flexible problem-solving environment. This computing environment will be accessed via high-speed networks from anywhere in the country—eventually, the world.

The Alliance is led by the National Center for Supercomputing Applications (NCSA) at the University of Illinois at Urbana-Champaign with major support from the National Science Foundation's Partnerships for Advanced Computational Infrastructure program. Additional funding for NCSA comes from the state of Illinois, the University of Illinois, industrial partners, and other federal agencies.

### Cover

The asteroid Castalia hitting the atmosphere of Venus. Researchers at the American Museum of Natural History, NASA, and the University of California, Santa Cruz, are using an Alliance SGI Origin2000 and community astrophysics code developed at NCSA to create such hypothetical impacts. The results will show researchers how long ago the planet's surface hardened and hint at the kinds of churning that could be going on inside Venus.



access



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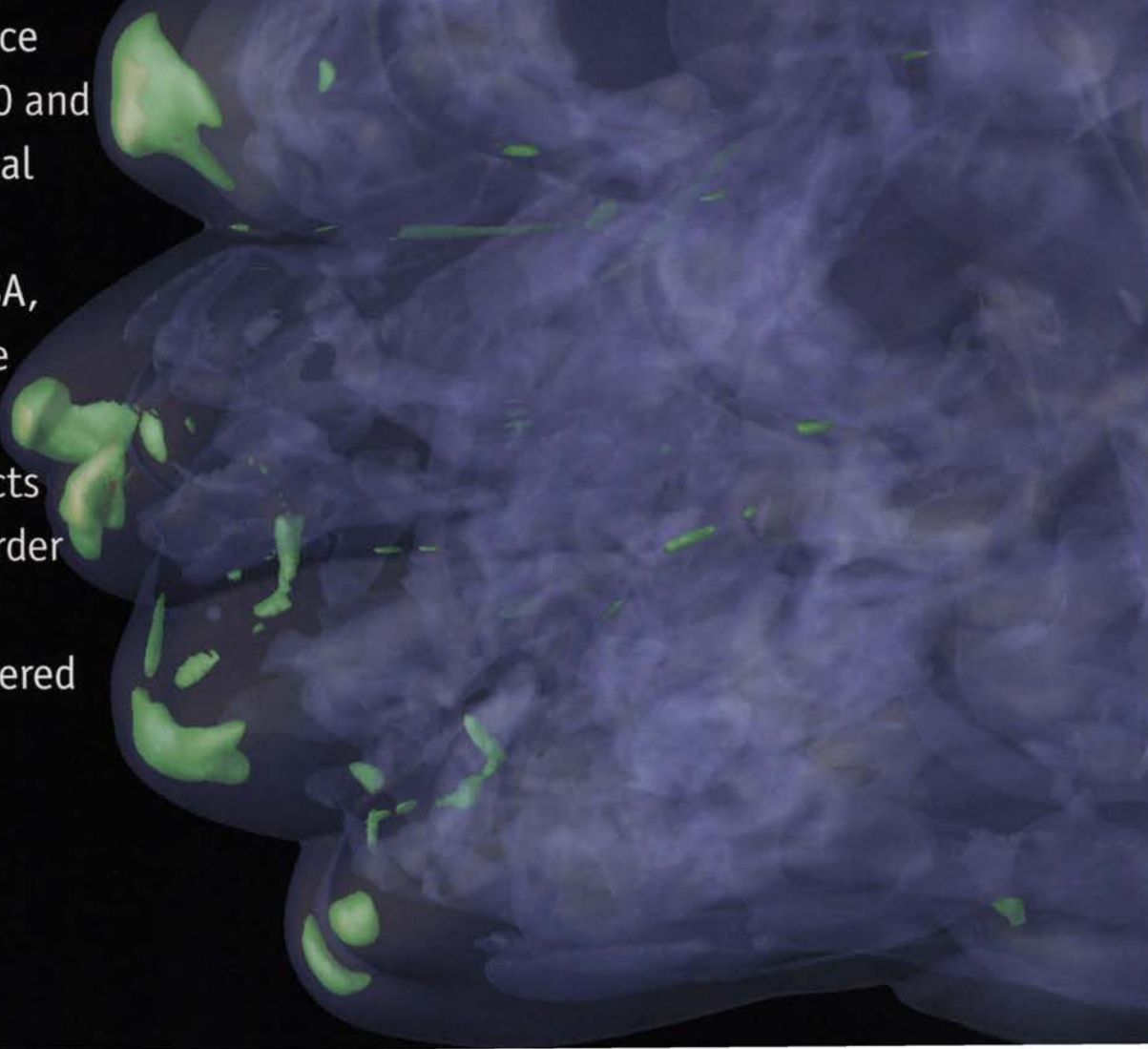
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# The asteroid diaries

by

Oliver Baker

With an Alliance SGI Origin2000 and an astrophysical gas dynamics code from NCSA, researchers are simulating asteroid impacts on Venus in order to deduce the age of its cratered surface.





**I**t happens so fast. For eons you're coasting at a cool 70,000 kilometers per hour on a seemingly endless circuit through space. You doze off for a moment. Suddenly you're riding a roaring shock wave through Venus' pea-soup atmosphere and lighting up like a second sun. You and your steadfast  $10^{20}$  joules of kinetic energy—worth 10,000 Titan-II thermonuclear missiles—are cashing in. And this isn't just a personal catastrophe. What about the planet? What about the atmosphere? What's happening?

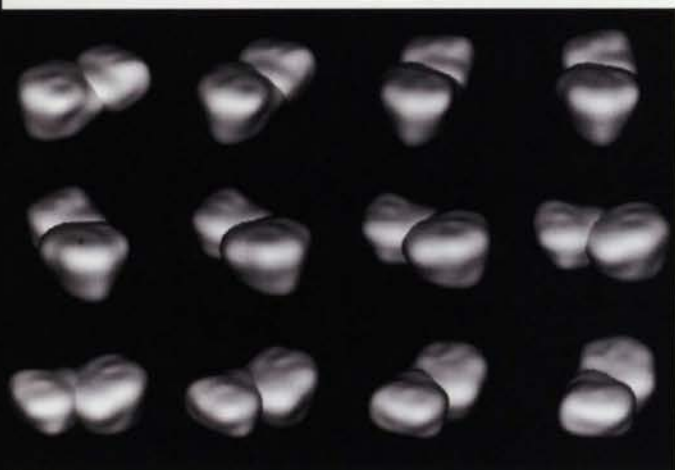
Answers to such burning questions may not help the asteroid, but researchers are after them nonetheless. Astrophysicists Don Korycansky, Kevin Zahnle, and Mordecai-Mark Mac Low believe that craters on Venus will tell them how long ago the planet's surface hardened—but only after they've learned what asteroids go through.

From radar images the Magellan spacecraft sent back in the 1990s, the researchers know the number and sizes of craters on Venus. From the observations of astronomers, they know the same statistics for asteroids, including how often different sizes hit Venus on average. But they can't connect the hits to the craters, because they can't predict how much oomph different asteroids have left—if any—after they encounter Venus' atmosphere. Once they understand what happens as asteroids come in, they will be able to calculate how many years of hits are really represented by the crater record on Venus.

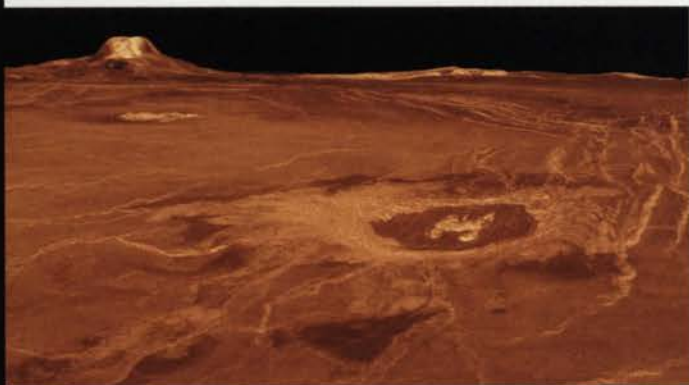
Zahnle, who works at the NASA Ames Research Center in Moffett Field, CA, devised a formula several years ago for how atmospheres sap the strength of asteroids. But he didn't have data with which to calibrate or test his formula for impactors of different sizes, speeds, and incoming angles—to name some of the parameters he believes will be key.

Zahnle might have set off with a notebook, binoculars, and a suit that could withstand a million-megaton blast for a billion-year expedition to Venus. Instead, he recruited Mac Low, a scientist with the American Museum of Natural History in New York, who crafted a software strategy for capturing on computer the detailed physics of atmospheric impacts. Zahnle also enlisted Korycansky, who built into the software a radar-imaged likeness of a real asteroid known as 4769 Castalia, which periodically crosses Venus' orbit. From his office at the University of California, Santa Cruz, Korycansky runs the team's impact simulations, employing an Alliance SGI Origin2000 supercomputer and NCSA's ZEUS community software for simulating astrophysical phenomena.





Computer rendering of Castalia based on Doppler radar data. Image courtesy of NASA/JPL.



A penetrating radar image of the cratered surface of Venus unobstructed by the atmosphere. Mapping Venus' surface was the primary mission of the Magellan spacecraft, which orbited the planet from 1990 until 1994. Image courtesy of NASA/JPL.

## How things shake out

Named for a nymph of Greek mythology, Castalia is an hourglass-shaped space rock that's 1.8 kilometers long that Korycansky describes as an ideal candidate for the team's simulations. By sending the irregularly shaped Castalia into Venus at different orientations, the modelers are able to assess how an asteroid's shape influences how well it penetrates the atmosphere. According to Zahnle's formula, furthermore, Castalia is more or less the smallest object Venus' atmosphere should allow through.

The simulations start with Castalia 100 kilometers above the cratered plains of Venus. Because the coordinate system of the team's computations moves with the asteroid's center of mass, animations of the data depict Castalia as if fixed in place even as the asteroid hurtles full tilt toward the surface. The resulting perspective is what you might see from a second asteroid diving in alongside.

As Castalia enters the atmosphere, a gauzy cloak of shocked Venusian air forms around it, and the rock starts lurching like a whiffle ball. On Castalia's leading surface, ripples appear, shift, swell, and break like waves. Then—FWOOSH!—the asteroid's face erupts, scattering rocky shards and billowing plumes of dust.

The growing undulations that undo Castalia are Rayleigh-Taylor instabilities, according to Korycansky. "The same thing that causes coffee to come out of a cup when you turn it upside-down," he explains. The instabilities appear whenever a light fluid (such as air) pushes a heavy one (such as coffee or a simulated asteroid). In the coffee situation, lumps give gravity handles on which to yank. For the asteroid, they are sheets that catch the supersonic wind, which tears apart the rock wherever it catches.

## Getting down to Venus

Though the animated data are vivid, the simulations do cut some corners. The virtual Castalia's descent is not fiery, and the computations currently leave out this physics. Real asteroids move too fast to absorb heat from the atmosphere and wouldn't exhaust much energy illuminating it, Korycansky says.

So far, the researchers have only modeled Castalia as a liquid, based on reasoning that is partly theoretical but partly practical. In principle, the aerodynamic forces generated by Castalia's cosmic plunge might make fast work of any material. In practice, assuming Castalia is solid makes the impact problem tougher and more computationally intensive. It also means speculation, Korycansky says, because no one knows whether asteroids are generally hard, powdery, or in between. And no one knows where cracks and fissures might run through Castalia in particular.



But the simulations are growing steadily richer in detail. The team ran its previous round of simulations on only four processors, but Korycansky is retooling the computations to exploit an updated and more parallel version of NCSA's ZEUS code. Mac Low predicts the team will soon be running simulations on hundreds of processors at once. Upcoming runs on NCSA's Origin2000 should give the team their first indications of whether the Venusian atmosphere deals differently with Castalia as a solid. Within a year, they expect to incorporate structural heterogeneity and flaws into the asteroid.

According to Mac Low, the more details that go in, the simpler the problem looks. In 2D runs with a spherical asteroid-like impactor, even minuscule adjustments of the impactor's velocity on entry sizably affected how much mass and energy reached the planet's surface. "In 3D, we took these lumpy, bumpy things, and we turned them around, and it made virtually no difference," he says.

Such results bode well for the ability of Zahnle's formula to extract the basics of an impact for a wide variety of asteroid shapes, speeds, and geometries of impact, Mac Low says. The formula closely captures how Castalia's cratering capacity would decline on a beeline descent through Venus' atmosphere, simulations show so far. Next the modelers will be simulating oblique impacts and trying larger asteroids.

With a formula calibrated to cope with the gamut of objects in the sky, the team will be able to enact impacts by the thousands and to discover how long Venus' craters have taken to accumulate. The result will tell them how long ago its surface hardened and hint at what kinds of churning could be going on inside the planet.

The goal is not far off, according to Mac Low. "We haven't calibrated it yet," he says, "but we're getting very close."

This research is supported by NASA. Images were rendered at the University of California, Santa Cruz. Erik Asphaug provided the shape model of Castalia. Mac Low is partially supported by a National Science Foundation CAREER grant.

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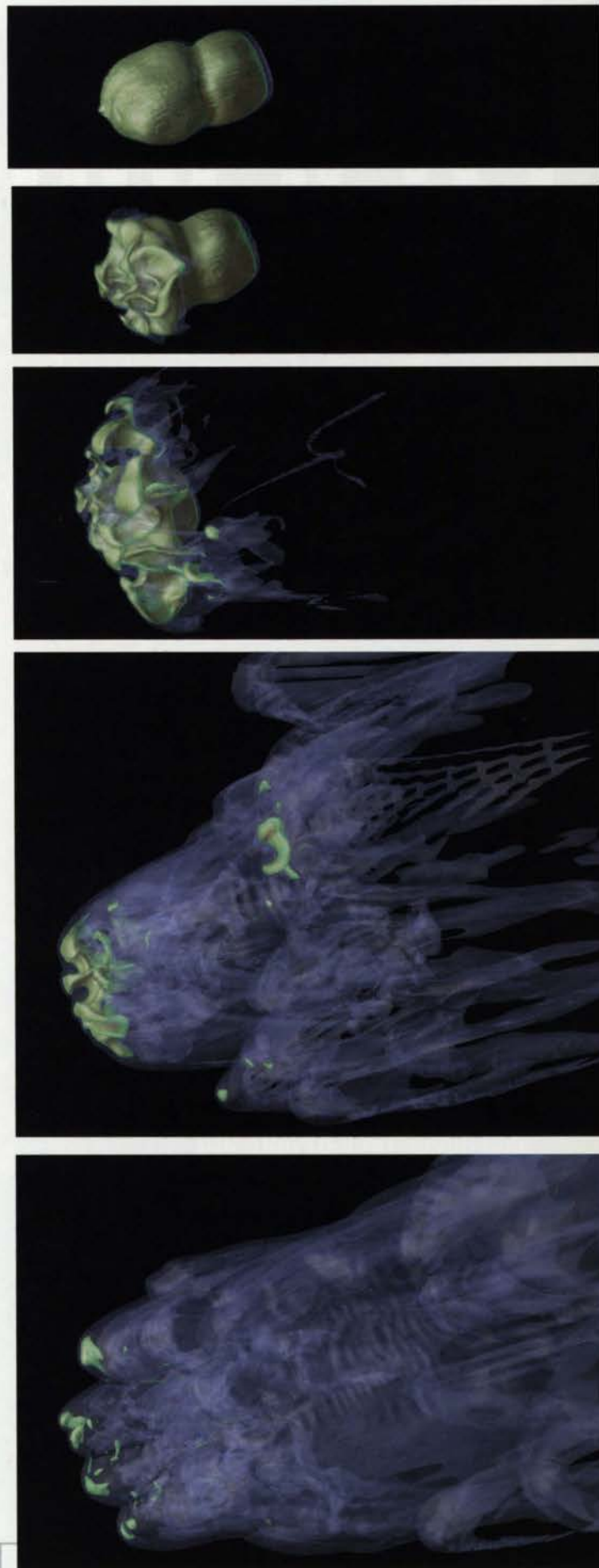
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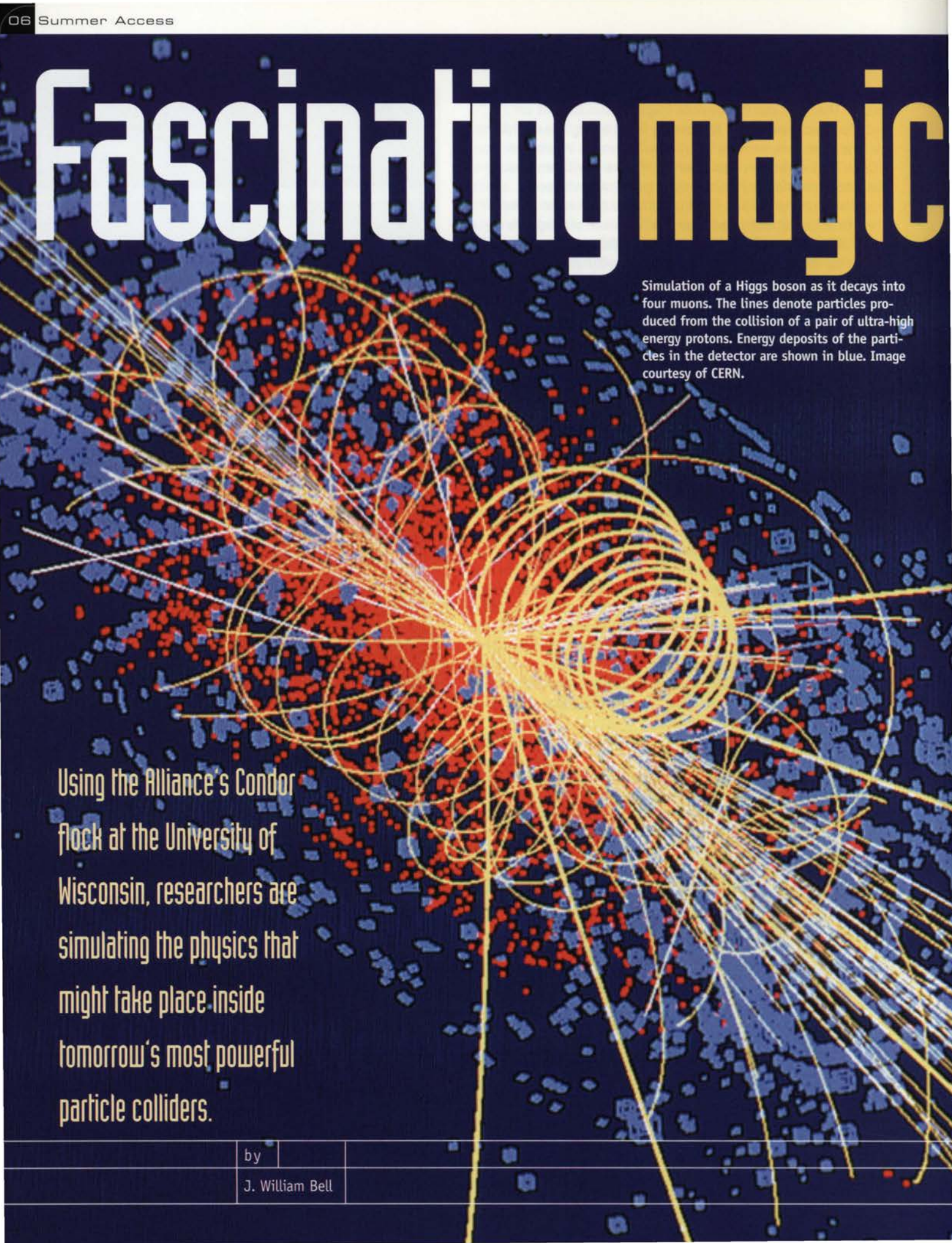
*Kevin Zahnle*



Simulation of Castalia hitting the atmosphere of Venus.



# Fascinating magic



Simulation of a Higgs boson as it decays into four muons. The lines denote particles produced from the collision of a pair of ultra-high energy protons. Energy deposits of the particles in the detector are shown in blue. Image courtesy of CERN.

Using the Alliance's Condor flock at the University of Wisconsin, researchers are simulating the physics that might take place inside tomorrow's most powerful particle colliders.

by

J. William Bell



**Albert Einstein** spent the last 30 years of his life chasing a unified field theory. The prospect of fusing the forces of nature held what he called a "fascinating magic." Despite his efforts, however, a single mathematical system bringing together electromagnetism, gravitation, the strong nuclear force that binds subatomic particles, and the weak nuclear force that governs atomic decay eluded him.

A unified theory still proves elusive. But the fascinating magic remains, and the search continues. As a part of the GriPhyN (Grid Physics Network) collaboration, a team of physicists and computer scientists at the California Institute of Technology (Caltech) is on the hunt for the Higgs boson.

This yet-undiscovered subatomic particle may well answer a few of the most vexing questions in high-energy physics: Is the current Standard Model of particle physics correct at extremely high energies? Is unification of nature's forces and matter even possible? Are proposed unification theories—like string theory in which the resonance of one-dimensional  $10^{-35}$  meter loops of energy is responsible for all the physical properties of the universe—on the right track?

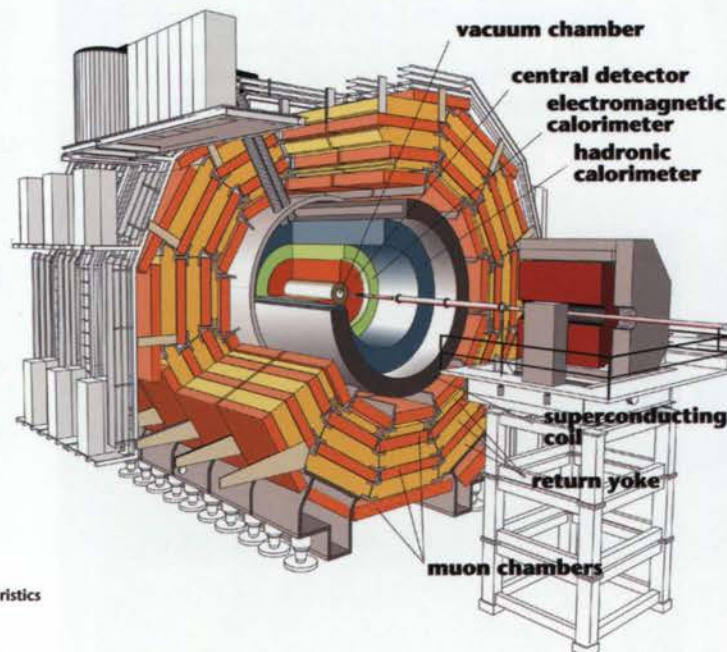
"Although our bias is to believe that it's unlikely, the right theory—the one chosen by Nature in our universe—might not be any one of those that has been thought of so far. Finding the Higgs would take us a long way toward finding out what the right theory is and whether or not nature is unified," says Harvey Newman, the physics professor who heads the Caltech team.

Using the Alliance's flock of Condor workstations at the University of Wisconsin, the team is simulating the physics in which the Higgs boson and other significant and elusive subatomic particles may hide.

### Physicist seeks boson

If tracking down a Higgs boson were easy, scientists would've found one by now. So how do you find a Higgs particle? Well, the Caltech team will use the world's largest particle accelerator, the Large Hadron Collider (LHC) being built near Geneva, Switzerland, by the European High Energy Physics Laboratory. The LHC is expected to go online in 2006. In the meantime, a massive amount of prep work is being done to manage and analyze the data and to perfect the collider's detectors. Catching a Higgs boson will require more than flipping a giant "on" switch.

The LHC is a circular vacuum tube in an underground tunnel about 17 miles in circumference. To flush out new subatomic particles, proton beams will be fired around the LHC at nearly the speed of light. The beams will cross at one of four interaction areas, allowing protons to smash into one another. The more focused the energy of those collisions, the smaller the component parts revealed. The LHC will be at least 10 times more powerful than any other particle accelerator ever built, and it is expected to be the first to produce a Higgs boson.

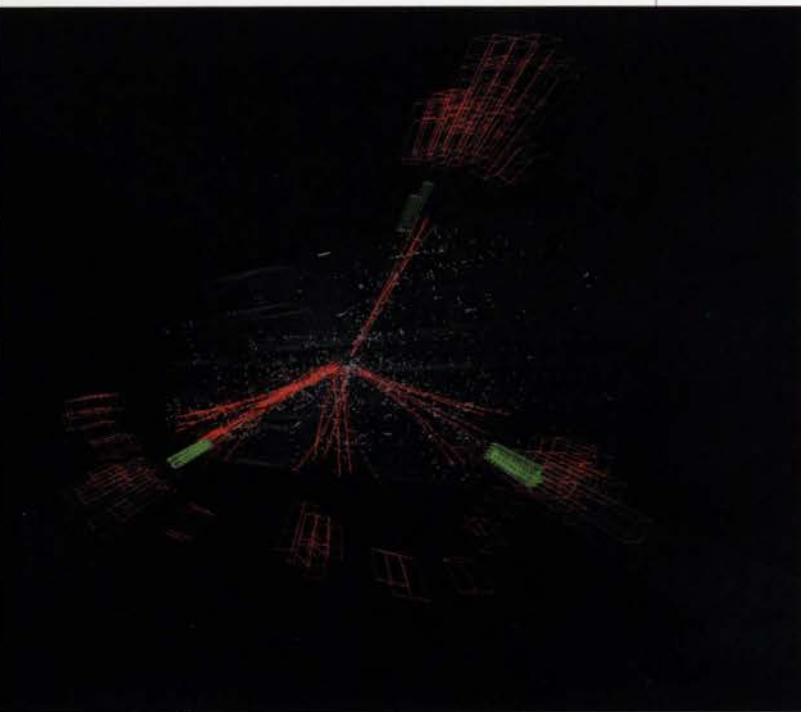


#### Detector characteristics

Width: 22m  
Diameter: 15m  
Weight: 14'500t

Schematic of the Compact Muon Solenoid.  
Image courtesy of CERN.





Multijet event of the sort that will be detected by the Compact Muon Solenoid. Jets are conical sprays of subatomic particles confined to a certain narrow width. Image courtesy of CERN.



Full-scale prototype of the LHC's 15-meter main magnets. Image courtesy of CERN.

When the LHC is running, proton bunches circulating in the tunnel will meet 40 million times per second, but at each meeting only about 20 proton collisions will occur. Still, that makes for about 800 million collisions per second. Most of the time, protons will only graze each other. The creation of a Higgs particle will require a head-on collision, and a variety of other conditions will have to be just right. But once in every 10 trillion collisions—which will be about once a day in the LHC's proton demolition derby—one should appear.

## Detector details

Data on the events that follow the proton collisions will be collected by giant detectors built around the LHC's interaction areas. These detectors will be filled with tubes of gases, silicon strips, and electronic sensors and encrusted with other electronics used to identify the particles produced.

The Caltech team's search for a Higgs boson will exploit a detector known as the Compact Muon Solenoid (CMS). The CMS experiment will have about 100 million individual sensors, all controlled and monitored by computer. "The CMS is the size of a very large house and built in layers like an onion," says Julian Bunn, a senior scientist at Caltech's Center for Advanced Computing Research.

Even the CMS will not detect the Higgs boson directly. Because the particle is thought to be incredibly short-lived, researchers will rely on circumstantial evidence. Higgs bosons are thought to decay in many different ways, or channels. In one channel, a pair of photons of a particular energy are created. The team will watch for a pair of electromagnetic radiation showers picked up by the detector. If these showers match the signature for the pair of photons, then the team will have evidence of a Higgs boson.

"The Higgs particles go only a couple of millimeters and last a fraction of a second before decaying to other particles. Our views of these tricky characters will always be indirect," says Bunn.

## Petabyte per second

A fundamental problem in high-energy physics is filtering through data. The LHC's detectors, for example, will track events that represent about one petabyte—or one quadrillion bytes—per second. A lion's share of these data are garden-variety events and particles that don't interest researchers. With its sensors honed to record only a very particular set of trigger events, the CMS detector will reduce this background by about seven orders of magnitude. Nonetheless, that leaves about 100 megabytes of data per second to digest.

A whopping 1.5 million CPU hours on Wisconsin's Condor system, which pools the idle processing time of general-purpose Linux workstations for use in large-scale computations, are already being used by the Caltech team to simulate LHC events related to the CMS detector. The team is also using an HP-Convex Exemplar system at Caltech and Linux clusters at Caltech and CERN to run the simulations.



"During peak processing times on Condor, we're submitting 600 jobs and have nearly 300 running," says Vladimir Litvin, a senior engineer in Caltech's high-energy physics program. "And the usual datafile from a production run is about one gigabyte. We need large amounts of processing power, storage space, and network bandwidth for our tasks."

The team has already simulated about 1.25 million LHC events related to the search for the Higgs boson, as well as another 1.25 million for other groups that will use the CMS detector to hunt other particles.

## Diverse challenges

These simulations give the researchers the tools to build two types of code for interpreting the LHC data. Reconstruction code uses energy information from the detector and tripped sensors to track the behavior of specific particles. In effect, it plays a game of 3D connect-the-dots—with as many as 5,000 points to consider—and divines the LHC events and the particles they produce. Analysis code, meanwhile, sifts through these re-creations, mining for particular events like the Higgs boson's photon decay.

"Reconstruction code gives us the properties of the event," says Bunn. "Analysis code lets us figure out the physics to determine the parameters of the events and see if those parameters match our hypotheses."

As researchers finetune these codes for the various events of interest, members of the NSF-funded GriPhyN collaboration—with an overarching goal of building petabyte-scale computing environments for diverse data-intensive projects—are meeting other LHC data management and analysis challenges. The Globally Interconnected Object Database project, for example, is addressing data storage and access problems like authentication and job handling. And a common data analysis toolkit and a common reconstruction code are being encapsulated in Java for use through Web browsers.

Once the LHC is up and running, more than a thousand scientists are expected to take part in one way or another. It's a big, diverse team working on a big, diverse project—a team that may capture the fascinating magic that Einstein sparred with for years.

This research is supported by the Department of Energy and the ongoing efforts of the entire CMS collaboration.

**Access Online** <http://access.ncsa.uiuc.edu/CoverStories/higgs/>

### For further information:

<http://www.cern.ch/LHC/>

<http://cmsdoc.cern.ch>

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Assembly of the Compact Muon Solenoid magnet system. Image courtesy of CERN.



# Parasites lost

by

Karla Harby



Protein structure research leads to the discovery that anti-osteoporosis drugs inhibit the organisms that cause malaria and other tropical diseases.



**Deadly** fevers have been known since ancient times. The Italians gave one of the more common fevers its modern name—mal' aria, or "bad air"—because it was widely believed that breathing the putrid vapors of swamps caused the affliction. In 1880 scientists found the real cause of malaria, parasitic protozoa of the genus *Plasmodium*. Eighteen years later, it was discovered that this malaria-causing protozoa is transmitted by the *Anopheles* mosquito.

Despite all that has been learned about malaria in the last century, nearly 300 million people suffer acute malaria each year, and at least one million a year, or about 3,000 people a day, die of the disease. According to the World Health Organization, a child dies of malaria every 40 seconds.

Malaria is, of course, a disease of the tropics and subtropics—of places with jungles, not cornfields. Yet the University of Illinois is the site of basic research conducted by chemist Eric Oldfield and tropical disease experts Silvia N. J. Moreno and Roberto Docampo that has led to an important advance in understanding malaria. Working with international collaborators, these researchers made the unexpected discovery that anti-osteoporosis drugs can inhibit the growth of *Plasmodium*. What's more, they found that these drugs can also inhibit the protozoa that cause several other diseases, raising hopes of a new drug strategy against a devastating list of illnesses.

This discovery might never have happened without computational chemistry—running quantum mechanical experiments on computers.

The researchers took advantage of NCSA's SGI Origin2000 supercomputer running the Gaussian 98 software. To make and confirm their key findings, the group used 35,000 service units of computing time in less than three months. "Over a year's allocation has just gone 'bing,'" Oldfield says. "Why didn't we ask for more? We didn't think it would require that much." He adds that they've been invited to apply for additional allocations.

## Beginning with the basics

The group's findings were published in the March 15 issue of the *Journal of Medicinal Chemistry*. Collaborators included tropical disease experts Julio A. Urbina, of the Instituto Venezolano de Investigaciones Cientificas in Caracas, and Simon L. Croft, of the London School of Hygiene and Tropical Medicine, as well as additional scientists and students from the University of Illinois.

But the work really began 30 years ago with basic studies into the structure of proteins. These massive organic molecules contain thousands of atoms that may be configured into many complex forms, as if they were birds or flowers folded from similar sheets of paper.

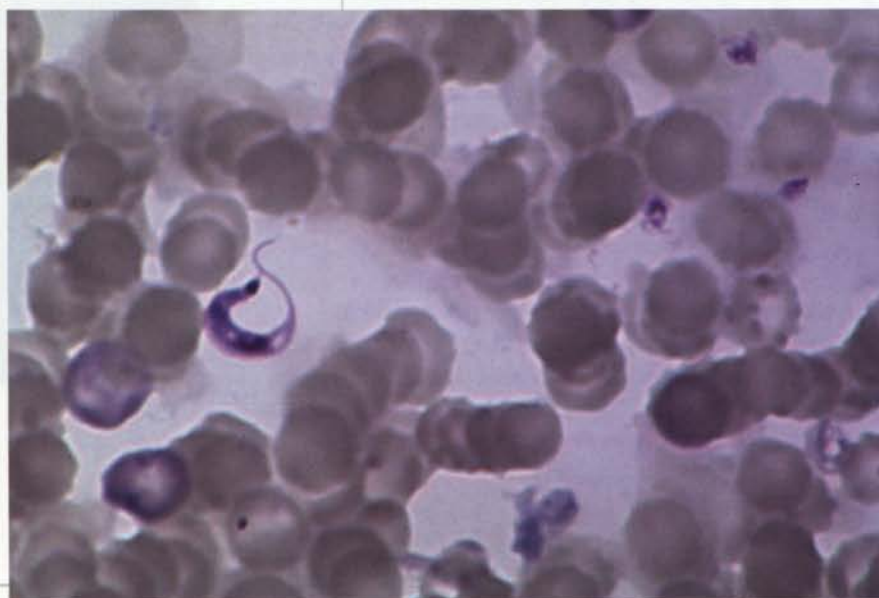
Oldfield and his colleagues demonstrated in previous research that carbon-13 NMR can be used to study proteins. They showed that experimental NMR spectra of amino acid residues in proteins are predictable with high accuracy by analyzing only small fragments of a protein. Then, using quantum chemistry calculations on NCSA's Origin2000, they overturned conventional ideas of how carbon monoxide binds with hemoglobin.



Adult female *Anopheles gambiae* mosquito, which can carry malaria. Photos courtesy of Sinclair Stammers for the World Health Organization Special Programme for Research and Training in Tropical Diseases.



Adult *Rhodnius prolixus*. This insect transmits the parasites that cause Chagas' disease in its feces, which are deposited near the site of the bite.



*Trypanosoma cruzi*, the parasite that causes Chagas' disease, in the blood.



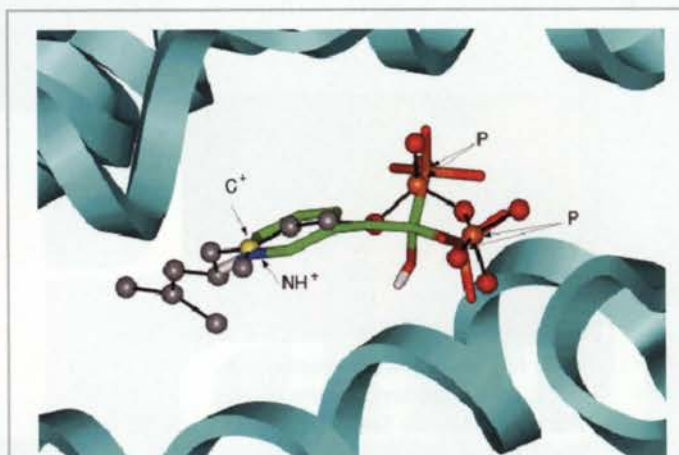


Diagram showing anti-osteoporosis drug Actonel® (green), superimposed on the normal substrate (gray) in the active site of the target protein (blue).

## Probing protozoa

Still, it's quite a leap from carbon monoxide to malaria. "It was totally fortuitous that we got into this area. We're interested in NMR, proteins, and quantum chemistry," Oldfield says now. He knew Urbina from their days in the United Kingdom and at the Massachusetts Institute of Technology. His NMR work suggested a useful collaboration with Urbina, who was visiting from Caracas, and they were joined by local parasitology experts Docampo and Moreno.

As they studied the chemistry of parasitic protozoa using NMR spectroscopy, they observed copious quantities of several compounds, including inorganic diphosphate and triphosphate, in the little pockets, or vacuoles, of all the major pathogens. This finding led to the idea that parasite growth might be inhibited in the presence of a stable analog of diphosphate. One such stable analog is nitrogen-containing bisphosphonate. The researchers were particularly attracted to bisphosphonates because they are already marketed to treat osteoporosis and other bone diseases.

Their bench science confirmed that bisphosphonates are indeed potent inhibitors of the organisms that cause malaria, as well as the less common diseases of African sleeping sickness, Chagas' disease, visceral leishmaniasis, and toxoplasmosis. The protozoa that cause encephalitis and diarrhea in patients, such as those with AIDS, who have compromised immune systems also appear to be inhibited by bisphosphonate in the lab.

To further explore precisely how bisphosphonates kill parasites, the Oldfield group proposed that the production of one phosphate compound in particular—farnesyl pyrophosphate or FPP—was being inhibited. FPP plays a central role in metabolism in a biochemical cascade known as the isoprene pathway, and the structures of the bisphosphonate drugs were proposed to be akin to those of a precursor to FPP.

So the group turned to Gaussian 98's quantum chemical calculations of the drugs' electronic structure and molecular geometries. From their results, they proposed how bisphosphonates interfere with the formation of FPP, which cells use to make sterols (as in cholesterol or ergosterol), and the signaling molecules cells use to communicate with each other. Working with tropical disease parasites in London, Croft was able to confirm that the drug target is the protein that makes FPP. Interestingly, the same target has been identified by other research groups studying the therapeutic mechanism of bisphosphonates in osteoporosis and bone disease, Oldfield says. Using NCSA's Origin2000, the researchers can now accurately predict the activity of their bisphosphonate drug molecules.

## Anatomy of a good drug

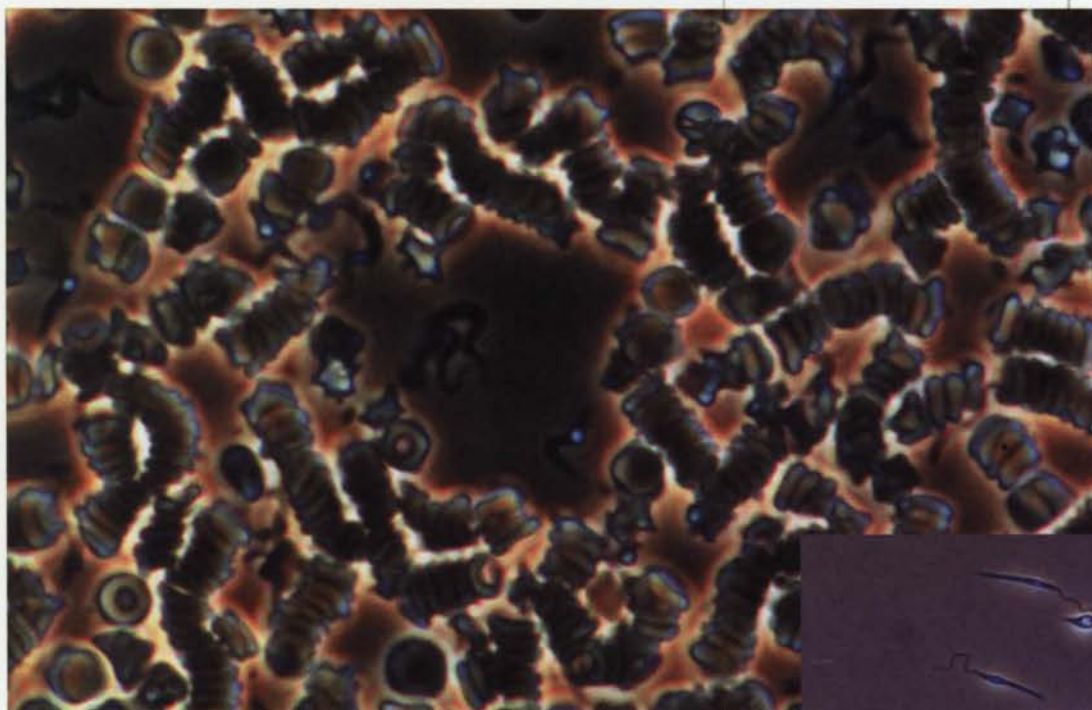
Whether bisphosphonates will serve as a new treatment for tropical diseases remains to be seen, but Croft is encouraged. "We've been testing drugs for at least 20 years, so we have a good idea of what looks like a good drug. When you see something good, you get a little bit excited about it," he says. "One has got to be skeptical as a scientist. There's a long way to go yet, but this has got the smell of an interesting story."

A good drug is one that kills parasites at low concentrations while simultaneously requiring extremely high concentrations to kill mammalian cells, Croft says. Once it passes that hurdle, a drug must then show efficacy in animals and later in people. Because existing treatments are so often ineffective, bisphosphonates—if they prove successful—would be an important advance in treating tropical fevers. Croft also finds it especially encouraging that bisphosphonates inhibit not only the malaria parasite, but also the parasites that cause the less common tropical diseases. Unlike malaria, these other diseases are too rare to attract much heavy investment in research and development.



Eric Oldfield, Silvia N. J. Moreno, and Roberto Docampo. University of Illinois.





*Trypanosoma brucei*, the parasite that causes African sleeping sickness, in infected mouse blood.

Docampo notes that because bisphosphonates are already used in humans, if they work for parasitic diseases, they could be put into clinical use relatively quickly. "They have already passed all the toxicity tests. They are known not to be mutagenic or carcinogenic," he says.

Docampo cautions, however, that even under the best scenario, routine use of bisphosphonates for malaria in people is a ways off. "I think we need to do more animal studies to establish the dose-response and which are the best compounds, and then after that, human trials," he says.

This research is supported by the National Institutes of Health.

**Access Online** <http://access.ncsa.uiuc.edu/CoverStories/parasites/>

**For further information:**

<http://www.who.int/tdr/>

<http://feh.scs.uiuc.edu>

<http://pubs.acs.org/journals/jmcmr/>

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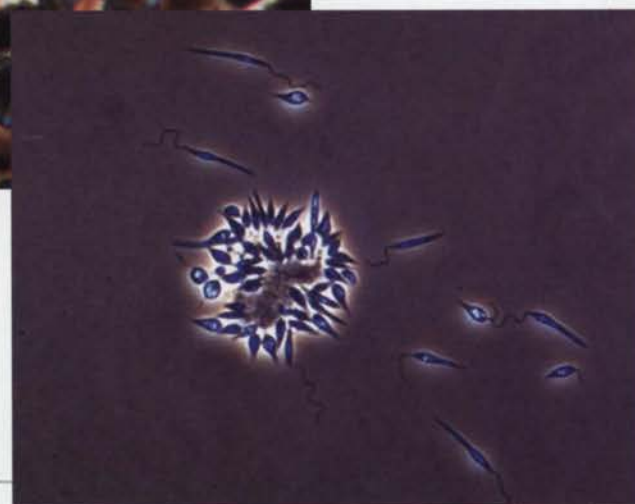
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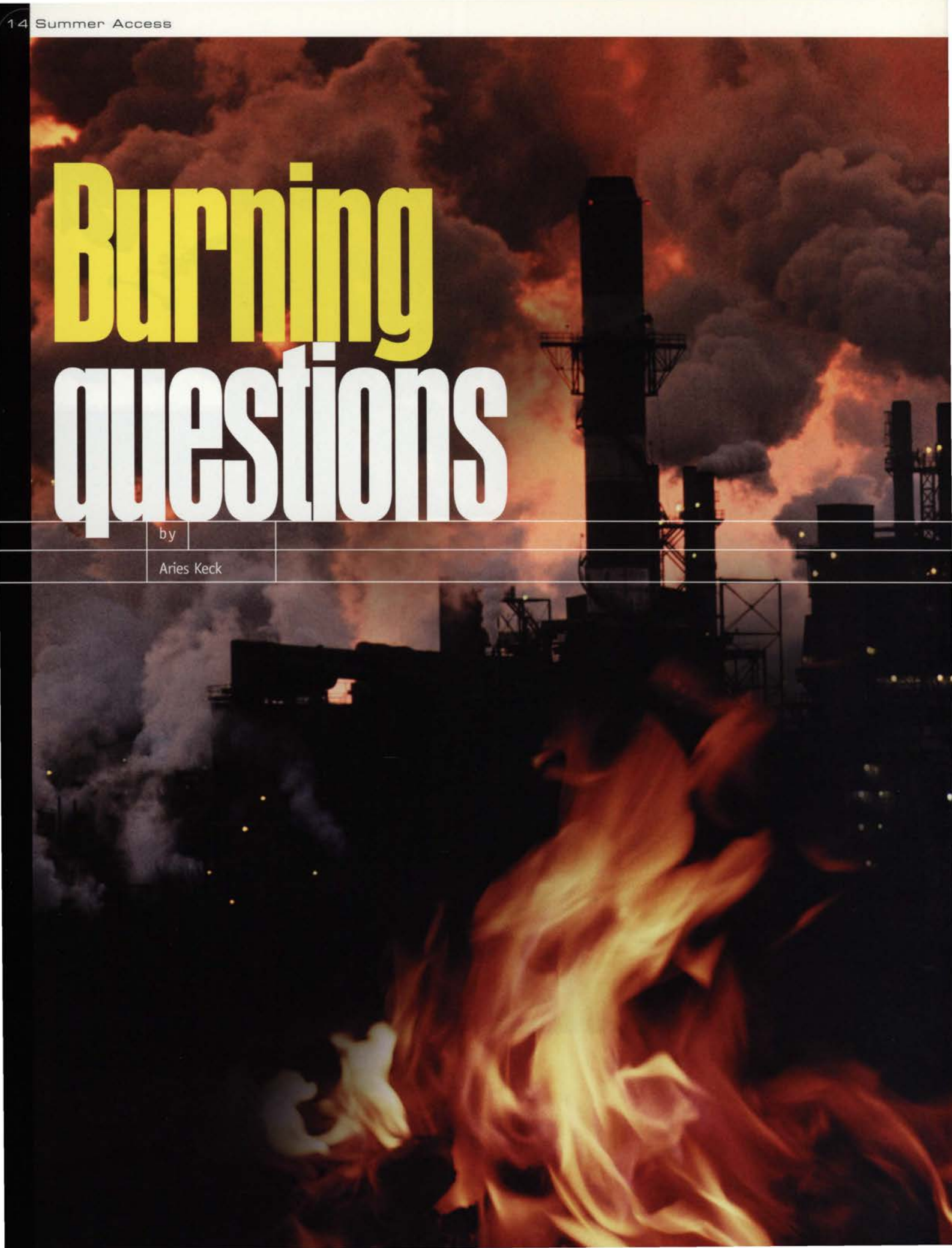
*Leishmania donovani*, the cause of leishmaniasis, in live culture.



# Burning questions

by

Aries Keck







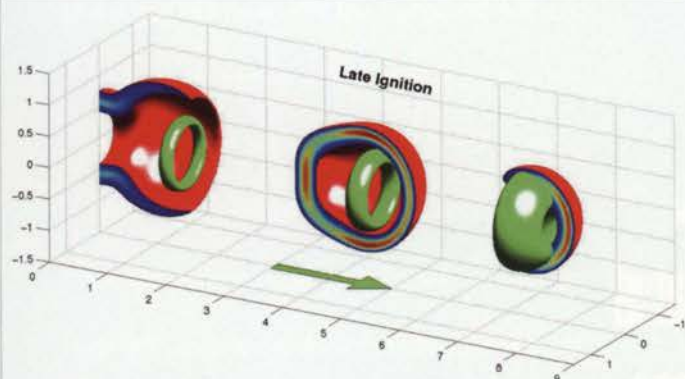
**Seminal computer models give researchers insight into how flames are created and how they are influenced by turbulence.**

**Fire** has always been a Faustian bargain. As humanity harnessed it for heat and energy our civilization blossomed and prospered. Fire has a dirty price, though. Soot, ash, unburned products, airborne toxins fill the air as the fire burns—in short, pollution is created. Our love affair with hydrocarbon-fueled combustion engines has made the downside of fire even more onerous. The implications of newer problems such as smog, acid rain, and global warming are still not fully understood.

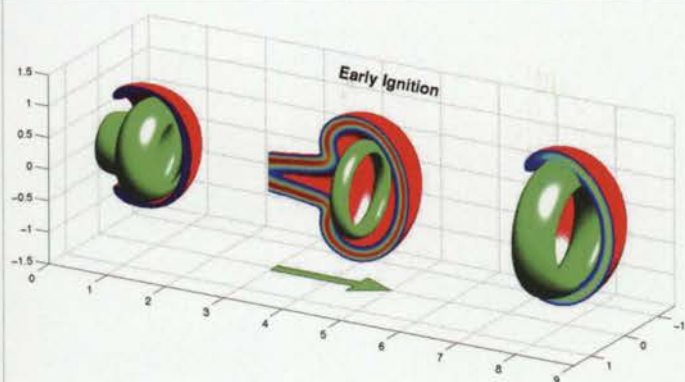
What makes fire so polluting is our lack of control over how fuel and oxygen mix together. Unburned fuel is released into the air as polluting hydrocarbons, and incomplete burning creates environmentally hazardous pollutants.

That's why aerospace engineer Cyrus K. Madnia and his team at the State University of New York at Buffalo are creating models that show how a flame is created and how its reactants and products whirl together in a dance of turbulent flows. Using these studies, the team hopes to help other researchers and engineers harness fire more efficiently and burn fuels more cleanly.





System in which fuel is added and then ignited. In this situation, the heat from the flame significantly distorts the vortex ring of fuel and, in the end, destroys the ring itself.



System in which fuel is ignited as it enters. In this situation, the flame produces less heat, and the ring of fuel is less distorted.

## Tornadoes of fire

Using NCSA's SGI Origin2000 supercomputer, Madnia's work at the Computational Fluid Dynamics Laboratory focuses on understanding flame-vortex interaction. This interaction causes pockets of reactants and products to swirl around flames in tornadoes of current and heat. These tornadoes, called vortical structures, are thought to be the dominant force driving turbulence in combustion.

"In most combustion systems, like aerospace propulsion, industrial furnaces, and power plants," Madnia says, "turbulence plays a key role in the mixing and reactions within the flames." Modeling vortical structures gives Madnia a better understanding of the ways turbulence influences the chemistry of burning fuels. This knowledge will help him, and other researchers, strike a very exacting balance in designing combustion systems. They will be able to find the most efficient flow of fuel for a given system.

Vortical structures are often affected by the method used to introduce fuel into a combustion chamber. For instance, when fuel is injected from a circular orifice, a donutlike shape develops in the fuel. This shape is called a vortex ring, and Madnia studies how a vortex ring forms when a hydrocarbon-based fuel combusts in air.

Using a model consisting of 49 chemical species and 277 reversible elementary reactions, his simulations predict the different ways the flame is created and how it interacts with the vortex ring of fuel. The result is a library of flames.

Some simulations are flames that are rich in methane, others are lean. Some flames create large amounts of polluting nitrogen oxide and soot, others produce very little. For example, one variation models a flame that ignites in the wake of a fully formed vortex ring of fuel. As this flame burns, the heat it releases significantly distorts the vortex ring. By the end of the burn, the ring itself is almost destroyed. (See top figure.)

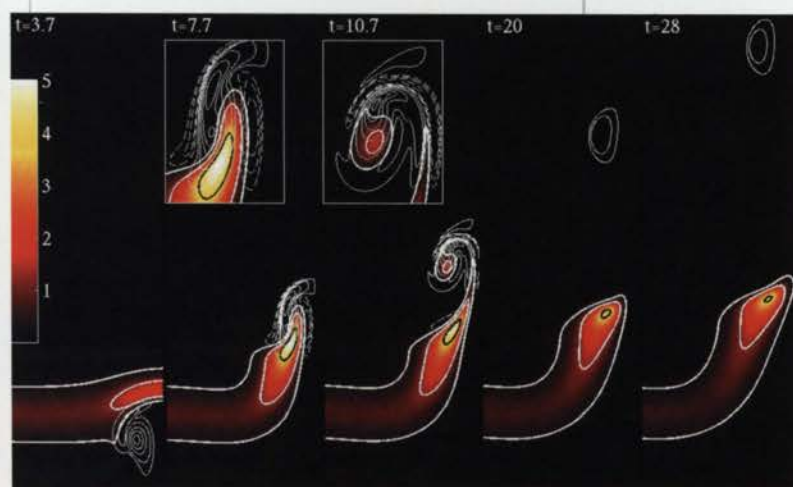
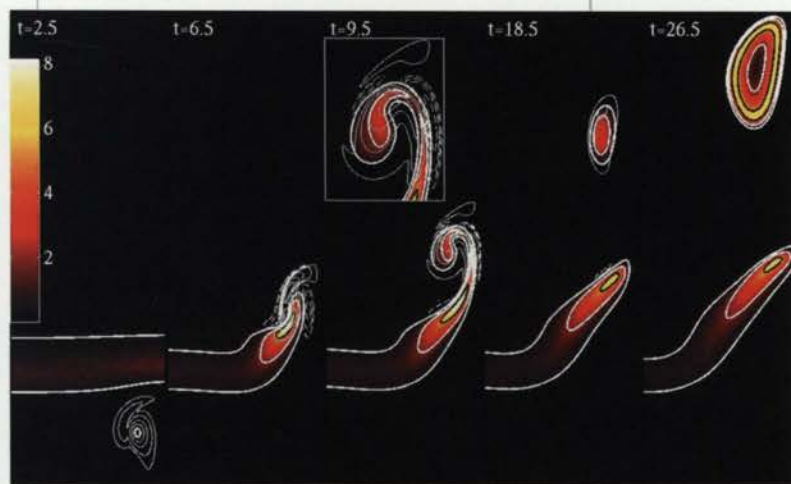
In another variation, the temperature of the entire system is increased, significantly altering its ignition dynamics. This time the ring catches fire as it's being formed, so less heat is released and the vortex ring of fuel is less distorted. (See bottom figure.)

Simulations like these, Madnia says, show how to alter a flame's characteristics to create more or less heat and less pollution. They let scientists tinker with ways to create cleaner flames.

## The basics are fundamental

Madnia's results are drawn from direct numerical simulations (DNS) used to dissect the burning vortex rings. They are possible only with a fully parallel computer code optimized for the SGI Origin2000 platform. The code performs very well—95 percent parallel efficiency is achieved in many of the simulation runs, according to Madnia. Due to the size and precision of the models, however, a typical simulation takes between 10 and 20 days running on 16 processors.





Simulations from Madnia's 'library of flames.'

When a run is completed, the simulations created on the Origin2000 are compared to experimental results obtained by W. J. A. Dahm's group at the Laboratory for Turbulence and Combustion at the University of Michigan. There are some limitations to a model's ability to capture the physics of a realistic combustion process, Madnia says, but the upside is that "DNS allows us a degree of control in isolating specific physical phenomena that is just inaccessible in experiments."

This level of control lets Madnia and his team use their simulations to answer the researchers' basic questions concerning the key physical characteristics of flames. Madnia says his next step will be to identify just how detailed these simulations can become.

While Madnia and his team focus on the basic character of flames, the implications of their work may someday answer questions in combustion-engine design. Hopefully, he says, the models could be used to replicate the basic features and details of flames in complex combustion systems.

"The ultimate goal of understanding this is to come up with models that are ingenious and that people in industry can use," Madnia says. He adds that, while this is basic research, it is also fundamental. "This is something that you do in research. First find the problem, then understand it, then add more and more difficulty."

In a decade or two he hopes his work will have a significant effect on combustion engines. "You see, first we understand this problem. Then later we model the chemistry, and then the soot. Which of course is of a great importance in terms of pollution and our atmosphere." This seminal research will allow engineers to look at models of how turbulence might influence the chemistry of a flame and how heat released from the flame might influence turbulence. Using this information, they will be able to change the parameters of different engine designs before the engines are produced.

This research is supported by the National Science Foundation and the Petroleum Research Funds administered by the American Chemical Society.

**Access Online** <http://access.ncsa.uiuc.edu/CoverStories/flame/>

#### Team members

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# Supercomputing to the rescue



by

J. William Bell

Work with NCSA's  
Private Sector Program  
on an Alliance SGI  
Origin2000 leads  
to a new industry  
standard for reducing  
the number of dropped  
cellular calls.



**Motorola** began testing its first mobile phone, called the DynaTAC, in the early 1970s. It was a monster, weighing in at two and a half pounds. The battery life was quite a burden, too—10 hours of charge time earned you only 35 minutes of talk time. The test phone used a single cell site perched atop a Manhattan skyscraper. Although DynaTAC was still 10 years from being commercially viable and other companies were building mobile phones, Motorola did win a critical race within the industry. In 1976 the company was granted a patent for the first practical cellular telephone system.

Today, cellular communication is a \$40 billion industry. There are more than 110 million cellular subscribers in the U.S. alone. And the phones fit in your pocket.

In May the NCSA Private Sector Program presented its 2001 Industrial Grand Challenge Award to Motorola's Jeff Bonta as he continues this tradition of innovation. The annual Industrial Grand Challenge Award honors breakthrough research enabled by a private sector partner's relationship with NCSA—research that will help ensure America's continued leadership in global business.

Bonta used thousands of hours on the Alliance's SGI Origin2000 supercomputer at NCSA to simulate real-world cellular systems. This work resulted in a new method of saving calls at risk of being disconnected. Known as rescue channels, this method will be part of the next-generation industry standard that will govern digital cellular systems in the United States and parts of South America and Asia. Rescue channels will be mandatory in all handsets, and—in an unprecedented move by the standard—setting body—they will also be mandatory in site equipment.

"If we were to actually go out and drive around the cities trying to capture enough data to be able to properly analyze the root causes of dropped calls, I'd be old and retired before we could get enough of that information," says Bonta, a senior member of the technical staff at Motorola. "By modeling cities on a supercomputer, I can run the simulation for 20 minutes of real time on 32 processors, and I can get the answers I need from a fairly busy system within 12 hours. If I had to run the same thing on a single processor system, it would be well over a week."

## Legacy of collaboration

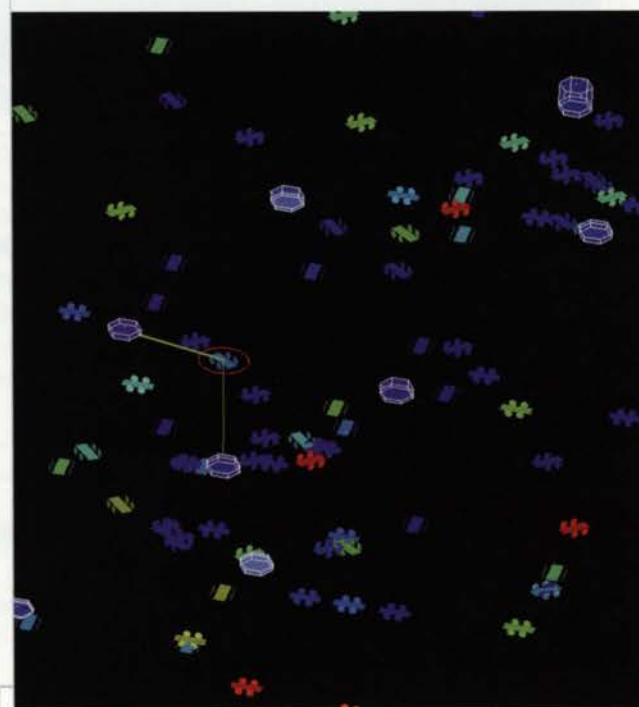
Motorola has been a member of NCSA's Private Sector Program since the late 1980s. Six years ago, another group of Motorola researchers received the Industrial Grand Challenge Award. In 1995 Gerry Labedz and his team developed massive computer models of early digital cellular networks using NCSA supercomputing resources and visualization software. The full-motion simulator, known as CMS, models cities configured with digital cellular infrastructure and mobile devices. It allows researchers to look at the radio connections between hundreds of cell sites and mobile units. Using the data produced, the researchers can evaluate system performance and call quality.

Bonta used CMS in the development of rescue channels.

"As we developed CMS, we realized that we were understanding the physical reality but that we needed to improve it. Improvements meant solving problems, getting rid of errors in the system," says Labedz, a

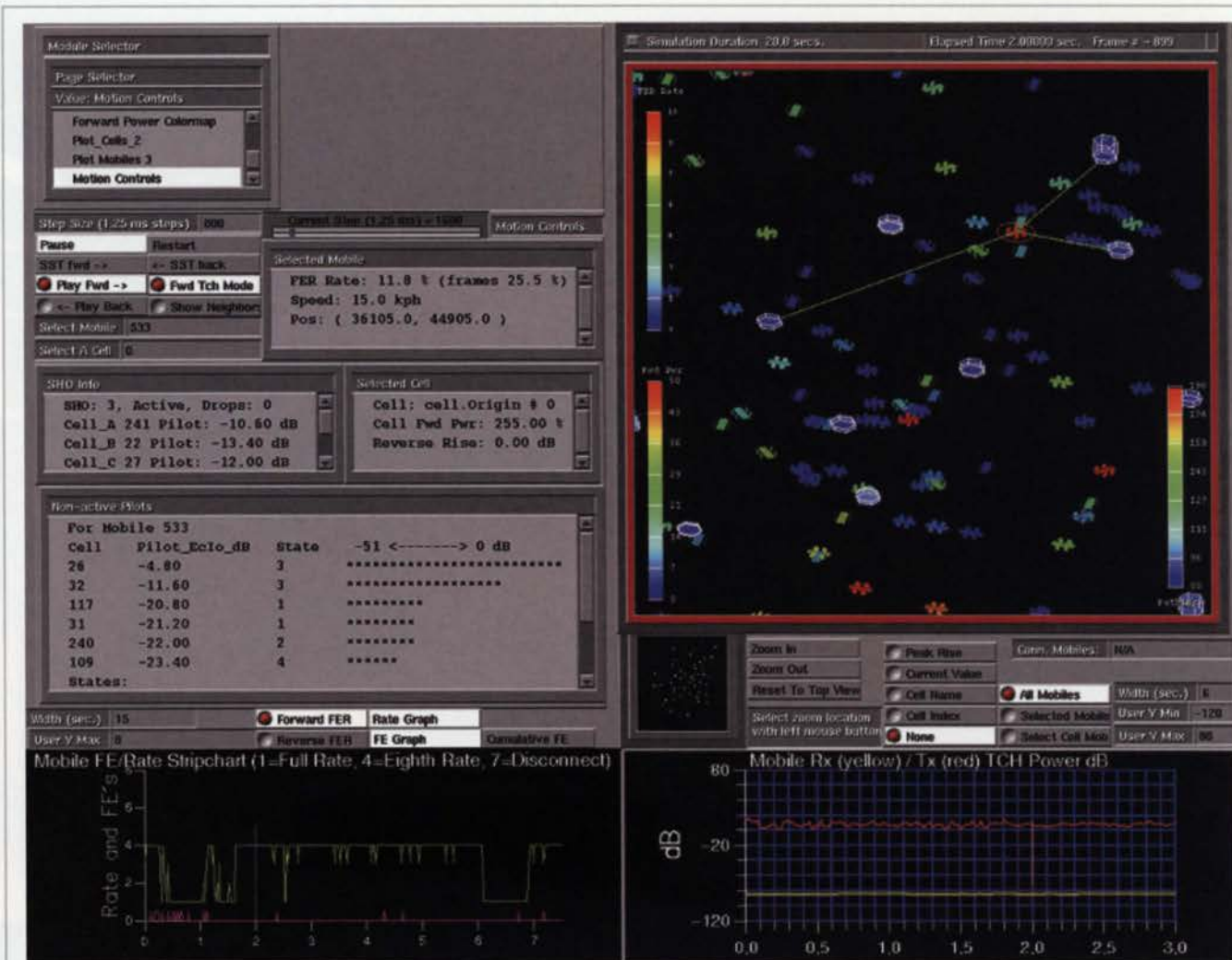


Developers of the first patented cellular telephone system with the Motorola DynaTAC phone.



Visualization from one of the numerous computer models used to design and perfect rescue channels.





Interface to the CMS simulation software.

principal member of the technical staff and Dan Noble Fellow at Motorola. "And that's where the rescue channels work comes in. Jeff was able to build a model from an idea that showed that his idea was really going to work without having to introduce it into a real, complicated cellular system."

"Motorola is an exemplar of what a company can do as a part of the Private Sector Program," says Dan Reed, NCSA's director. "For more than 10 years in the program, using a whole succession of computer technologies at NCSA to develop generations of new products, Motorola has gained advantage in the marketplace. Rescue channels is only the most recent fruit of this long legacy of collaboration."

## Rescue channels explained

To understand rescue channels, you first have to understand how calls are handed off from one tower to another in a traditional cellular system. When a cellular call is established, the subscriber's mobile is connected to a cell station or tower over a radio channel. As the mobile unit moves through an area, the quality of its connection with this station is in flux. The mobile constantly monitors signals from

other stations, looking for a new station that might provide a better signal.

If the mobile finds a neighboring station that provides a better signal, it requests a "hand off." In a hand off, the mobile sends a message to its original station saying that it has found a neighboring station that it would like to switch to. The original base station sets up a radio channel on the new station and gives the mobile permission to switch to that channel. The mobile then has a new, better connection to a new station, and the subscriber's call continues.

However, this system of handing calls off is susceptible to failure.

As the signal to the original station becomes weaker, interference can interrupt communication between the mobile and the station. If the mobile's request for a hand off does not reach the station or if the new channel information does not reach the mobile, interference can overwhelm the signal. The call can be dropped.

"Rescue channels allow the system to prepare for what might be inevitable. In any cellular system, there is going to be some level of interference. What we try to do is get the system to anticipate what might happen and make plans for getting around that particular problem," says Bonta.





Visualization from  
Gerry Labedz's early  
CMS simulations.

With rescue channels as a part of the system, the base station and the mobile agree ahead of time on what to do if something goes wrong. Rather than waiting until the signal is weakened, the mobile and the station establish rescue candidates at the beginning of the call and any time there is a hand off during the call. Channels on neighboring stations are reserved for the mobile before a hand off is necessary. And—in a further improvement over the current system—the mobile is empowered to select the station to which it will hand off. It can even initiate that hand off on its own.

That way, even if interference overcomes the original signal, the mobile can make the switch to the new station on its own—the channel has already been reserved, permission has already been granted, and a substantial number of calls are saved.

This elegant solution takes less than a second to execute, requires no changes to physical infrastructure, and is totally transparent to the customer.

### No more 'Are you there?'

Bonta's rescue channel concept is part of the larger 5NINES initiative underway at Motorola. 5NINES—as in 99.999 percent end-to-end service availability—is a companywide drive to make cellular service more reliable than your home phone. This goal will translate into about five minutes of downtime per year for a customer and will effectively eliminate the most common question plaguing cellular communication. No more "Are you there?" shouted into your mobile as you drive along.

5NINES is crucial to the company's future competitiveness, and it will require continued support from NCSA and the Alliance.



Jeff Bonta,  
Dan Reed, and  
Motorola Labs  
Vice President  
Frank Yester at the  
Industrial Grand  
Challenge Award  
ceremony.

"Some time ago, Motorola learned that it couldn't do it all," says Dennis Roberson, Motorola's Chief Technology Officer. "There are expertise areas that should be drawn upon instead of developed within the company. The simulation and modeling capabilities of NCSA in both their human manifestation as well as their manifestation in computational power and infrastructure really do provide Motorola with a great partnering opportunity."

The rescue channel concept was developed at Motorola Labs, the advanced research arm of Motorola, Inc.

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# New age agriculture



by

Karen Green

Remote-sensing technology and innovative data mining methods lead to new and better farming techniques.



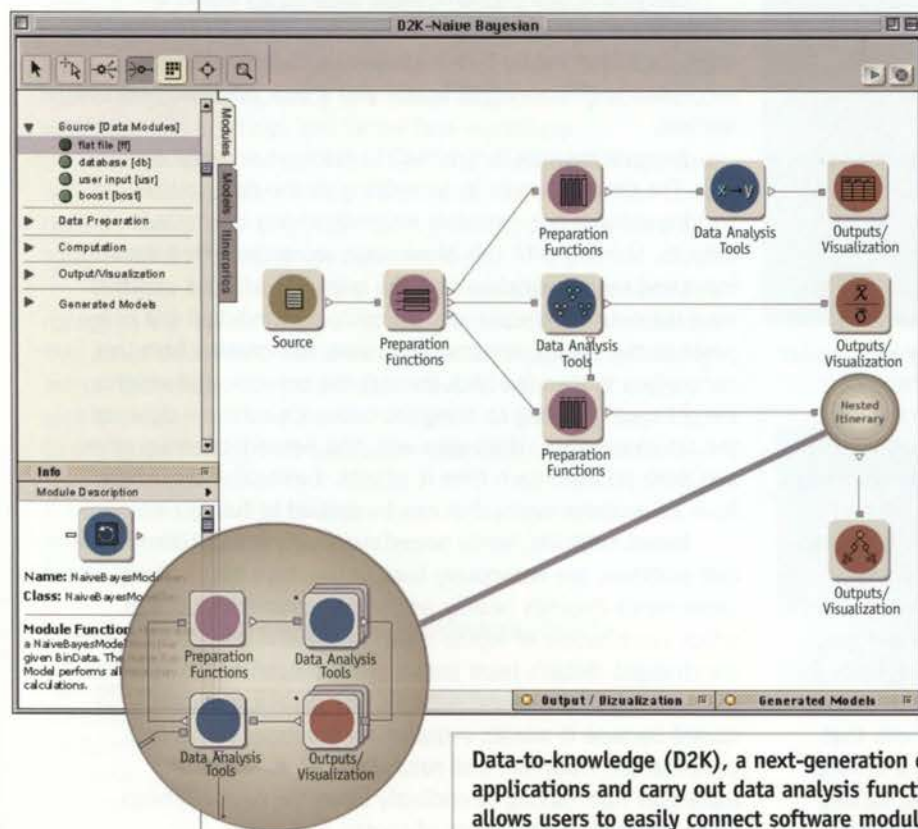


**Today's** farmer can choose from a wide range of precision farming tools, including machinery that makes targeted treatments of crops possible. Such specialized equipment fertilizes and controls pest problems only where needed and offers more than time and cost savings. Chemical runoff from farms is a major source of water pollution in agricultural areas, sometimes threatening water supplies, rivers, and lakes. Precision farming can reduce the use of chemicals without threatening productivity.

However, a lack of high-quality data and the challenge of converting data into useful information have slowed adoption of new farming techniques. While some farmers have accumulated a lot of data about their fields over the years, collection methods and data quality vary. Farmers need more than mountains of data; they need useful information.

Lei Tian, an assistant professor of agricultural engineering at the University of Illinois at Urbana-Champaign, aims to give farmers the data they need to bring agriculture into the Information Age. Tian and his research team at the U of I-based Illinois Laboratory for Agricultural Remote Sensing use global positioning systems (GPS) and remote sensing systems to collect high-quality data about crops, pests, and related issues. Working with researchers in NCSA's Automated Learning Group (ALG), Tian and his team pore through existing data to find meaning and relationships that can shed new light on problems in agriculture and promote new farming practices.

"In the normal field, only about 20 to 30 percent of the field has weed problems, which means you should only have to spray 20 to 30 percent," says Tian. "But in reality, we spray 100 percent. Farmers just don't have the information they need for precision farming."

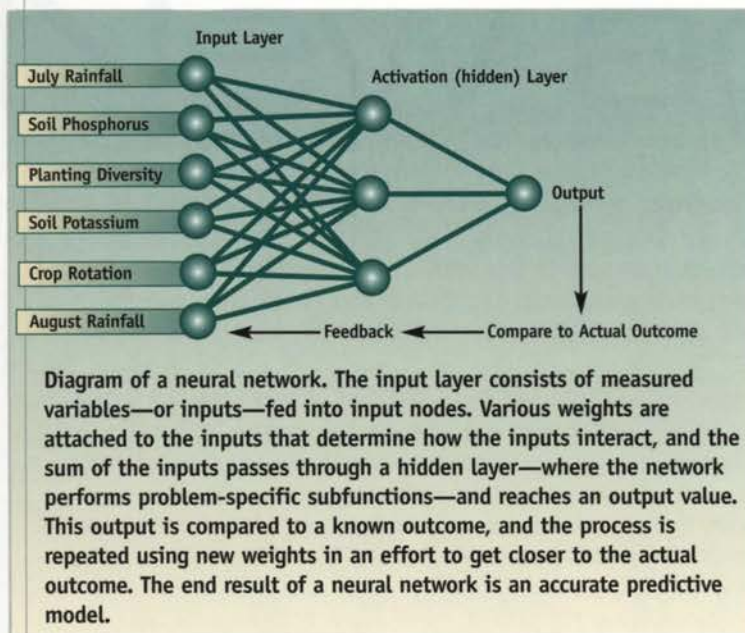


## Better data through new collection techniques

The first step in giving farmers more accurate information is using cutting-edge tools to gather very detailed information. At the U of I's experimental research fields a few miles east of campus, Tian uses GPS to pinpoint locations of problem areas in fields. High-resolution images taken by remote sensing systems help to identify types of problems. Airborne sensors created by NASA divide the data into as many as 250 bands of spectral reflectance and use reflection from the sun's radiation to determine characteristics of the soil or plant canopy. With these sensors, each spectral band can be used to identify a specific problem or characteristic, such as an area of pest infestation or areas with very high or low moisture levels. The GPS and remote-sensing technologies are then combined to create detailed maps to identify problem areas and problem types.

**Data-to-knowledge (D2K)**, a next-generation desktop workspace used to create data analysis applications and carry out data analysis functions. The D2K visual programming environment allows users to easily connect software modules to meet their needs. The green source module on the D2K desktop brings data into the D2K environment. Purple modules represent specific preparation functions, such as rule simulation, that set the parameters for data analysis. Blue modules represent data-analysis tools such as a neural network, a decision tree, or a genetic algorithm. Orange modules represent various outputs or visualizations that result from the analysis. Possible results include table data, descriptive statistics, or a visualization of a predictive model. The nested itinerary module groups together modules that are designed to work together. Software modules can be stored in a central repository and used by other researchers. D2K works with the Globus toolkit for distributed computing and will be an important analysis tool in the Alliance's developing computational cyberinfrastructure.





"Obtaining and analyzing data are the bottlenecks in the traditional system," says Tian. "The cost of obtaining information through traditional means, such as sampling for soil fertility or pest presence, is expensive and time consuming, and the data collected is relatively sparse."

In a field of 50 acres, Tian explains, a researcher traditionally takes one soil sample for every three acres to gather data about soil and growing conditions. That totals about 15 soil samples for the 50-acre field. "If you have remote sensing images, every pixel in the images covers about five meters of the field. For that same 50-acre field, you get 126 samples," he says.

Tian began collaborating with Michael Welge, head of NCSA's ALG, through the NCSA Faculty Fellows Program, which provides grants to U of I faculty to work with staff and use the resources at NCSA. He knew that new data collection techniques required new data analysis techniques, and Welge's team of researchers specialize in cutting-edge data analysis called data-to-knowledge (D2K).

Tian's first project with NCSA involved analyzing 30 years' data accumulated on the U of I campus at the Morrow Plots, one of the oldest and most famous experimental crop fields in the country. Crop systems specialists routinely analyze Morrow Plots data using traditional statistical analysis methods that involve random sampling, averaging, and analyzing a limited number of variables. The ALG, using D2K techniques, tackled the data with a hybrid data mining method that couples a genetic algorithm with a neural network.

## Predictions that power change

The neural network process develops a model that can be used to predict outcomes of future events. With the Morrow Plots data, Welge's research team developed a model that predicted how 15 variables—including rainfall, temperature, soil moisture, and fertilizer—influenced crop yields. Their analysis of the data revealed some insights that previous data analyses had not. Most importantly, the models showed that rainfall amounts—

especially rainfall during the long, hot July days—was by far the most important influence on yearly crop yields. Rainfall was more important than amounts or types of fertilizers used, crop rotation cycles, or nitrogen levels in the soil. Such knowledge discovery techniques lead to accurate predictions. The ability to accurately predict outcomes can change how farmers practice their trade.

A neural network is a nonlinear function that maps multiple input variables to possible outputs in a way that is similar to a biological nervous system. Whereas a nervous system has neurons that take in sensory data, a neural network has inputs that pass through network nodes. Instead of axons and dendrites carrying messages between nerve cells, a neural network has weights and paths that determine how inputs interact and influence the final output. A multilayered neural network starts with an input layer and ends with the output layer. In between are one or more hidden layers that allow the neural network to construct problem-specific subfunctions needed to solve difficult problems.

Every node in a neural network sums up its inputs and passes the sum through the nonlinear activation function to reach an output value. Each node passes its information in succession until the output layer—and a final prediction—are reached.

A neural network is "trained" to reach an accurate prediction. The process begins by scrambling all the data so that nothing remains but a random mapping among inputs and outputs. Starting with this blank slate, researchers feed known input and output variables into the system. The input variables start the network process, and an outcome is reached and compared to the known, or actual, outcome. Information from this comparison is then fed back through the network, and weights are changed gradually to bring the network's outcome closer to the actual outcome. If all goes well, the network becomes more and more accurate each time it adjusts. Eventually researchers have an accurate model that can be applied to future problems.

Neural networks, while powerful enough to solve many difficult problems, are notoriously hard to use, says Welge. Their performance depends heavily on control parameters, such as which combination of inputs is considered and how fast weights are changed. Welge's team uses a genetic algorithm to optimize the accuracy of the neural network. The genetic algorithm—so named because it mimics evolutionary processes like genetic combination, mutation, and natural selection—saves the researcher from having to endlessly rerun the neural network using different combinations of control parameters.

"What you are looking for is the best combination that provides the best predictive model," explains Welge. "In this case, we ended up with an optimized model that allows you to predict future crop yields."



## Data into meaning

Analyzing the Morrow Plots data was a success and showed that worthwhile information could be extracted even from older data that varied in quality from year to year. Now Tian wants to combine the high-tech data collection techniques made possible by GPS and remote sensors with ALG's data-mining expertise and tools.

"We realize how important high-quality data is and how much information you can extract if you have the data," says Tian. "We want to create a database of high-quality data that can be used well into the future."

Tian and his research team, including the ALG researchers, plan to use the U of I experimental fields to develop an analysis environment in which tiny, remote sensors are used to monitor plant growth, moisture levels in the soil, root growth, and other growing conditions. ALG's role will be to find meaningful relationships that inspire better agricultural practices.

"What we bring to this laboratory is the ability to extract meaning from their data," says Welge. "We help them understand relationships between things like soil temperature and moisture levels and the amount of growth over time." Understanding these relationships, he adds, leads to a better diagnosis of problems, better farming practices, and better farm machinery.

Tian envisions the day when farm machinery will be equipped with their own remote sensors. These machines will react to conditions on the spot as they move through fields, deciding when to spray or what spacing to use between seeds.

This new age of agriculture will do more than bring new technology to the world's farmers—it will give them detailed information about their fields. While the Industrial Revolution eventually led to mechanized farms that often leave farmers out of touch with their land, the information revolution could bring them back to the land in a way that hasn't been practical for decades.

This research is supported by the Illinois Council for Food and Agricultural Research, the NCSA/UIUC Faculty Fellows Program, and the U.S. Department of Agriculture.

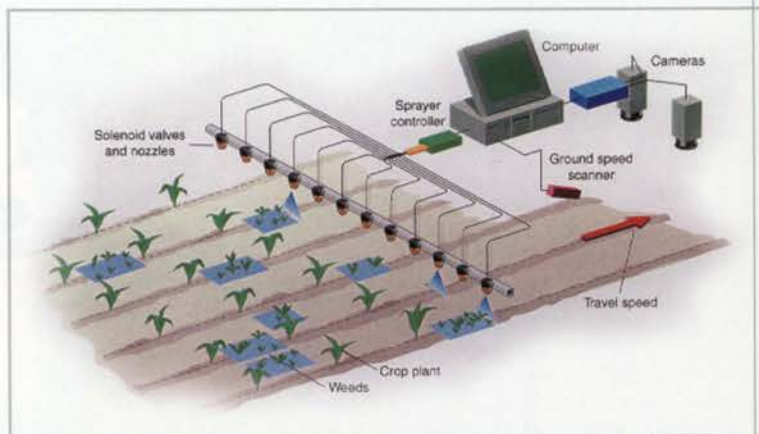
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### Team members:

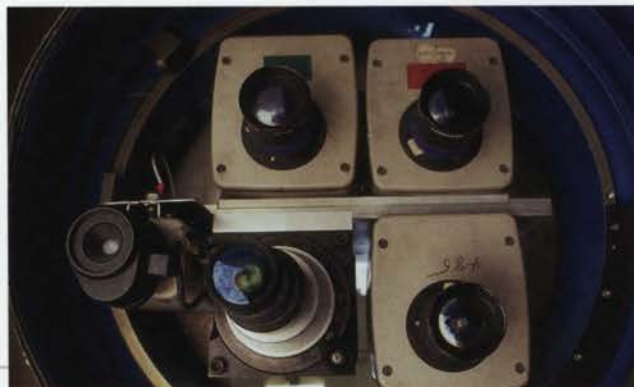
Don Bullock  
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Michael Welge  
Jim Westervelt

### For further information:

<http://www.age.uiuc.edu/remote-sensing>  
<http://www.ncsa.uiuc.edu/ALG/>



The future of farming. Farm equipment may someday use its own remote sensors. The machines will react to conditions on the spot.



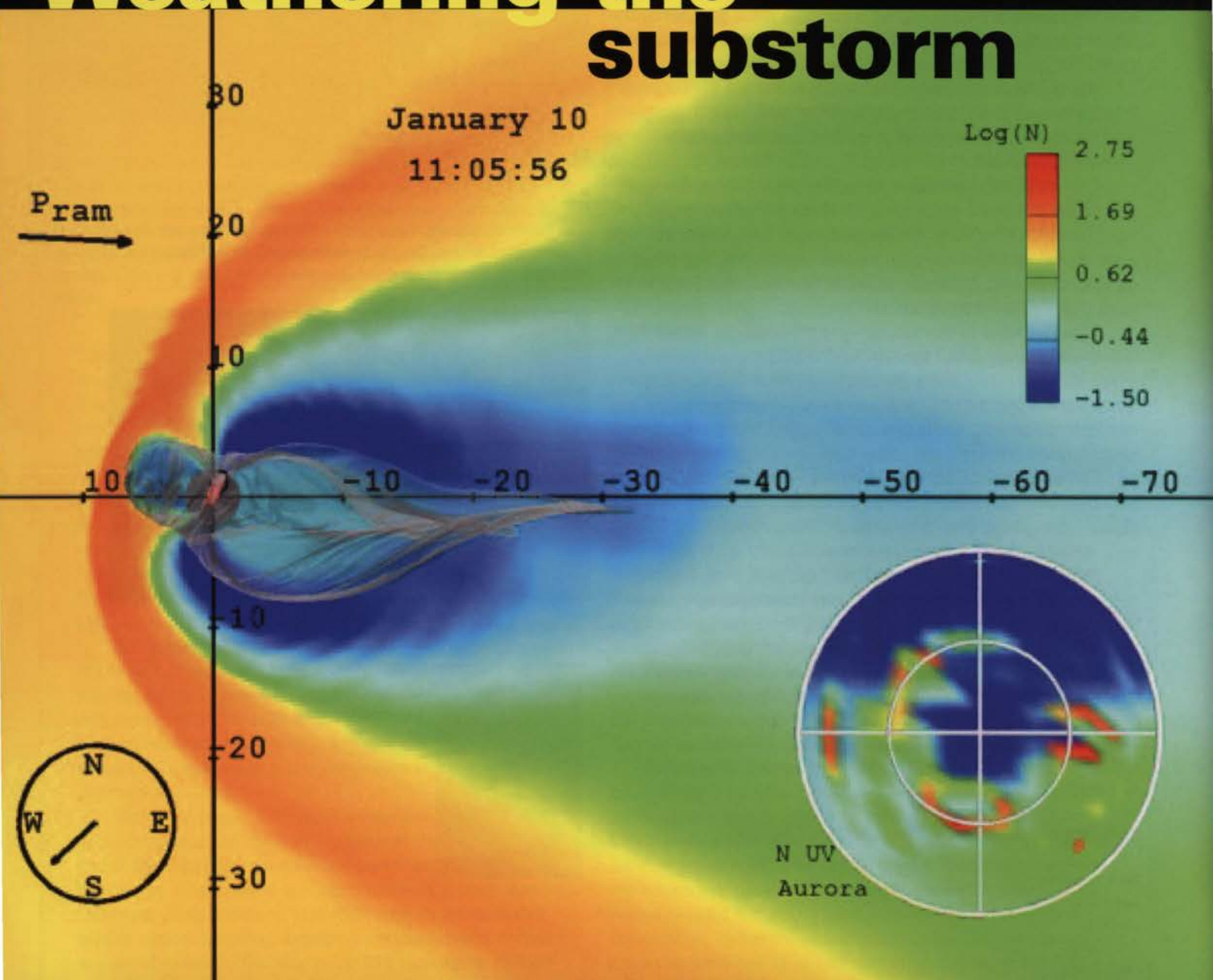
Sensing device.



Lei Tian.  
University  
of Illinois.



# Weathering the substorm



by

J. William Bell

Realistic views of the earth's magnetosphere during substorms are key to understanding this complex system.

Visualization of a magnetic storm in January 1997 that was associated with satellite failures.



**From** 60 to 60,000 miles above our heads, the earth's magnetic field is king. In this region, known as the magnetosphere, geomagnetism dominates the physics of the processes that take place. But, as any chess player can tell you, a king often lives and dies at the caprice of other subjects. A queen can sweep across the expanse and really crimp his style. Our solar system is no exception, as our matriarch, the sun, constantly influences the earth's magnetic field.

Magnetospheric substorms, brought on by solar activity, can dump quadrillions of joules of energy into the earth's upper atmosphere in about a half an hour. And these substorms occur two or three times a day.

Using the Alliance's SGI Origin2000 supercomputer at NCSA, a team of physicists is modeling the fine points of this cosmic chess match, building facsimiles of real substorms based on data from earth-bound and space-borne instruments. The team includes Michael Wiltberger and John Lyon of Dartmouth College, Charles Goodrich of the University of Maryland, and Tuija Pulkkinen of the Finnish Meteorological Institute in Helsinki. Their work is delivering some of the first realistic global views of substorms in progress. It will also prove critical in the ever-progressing field of space weather forecasting.

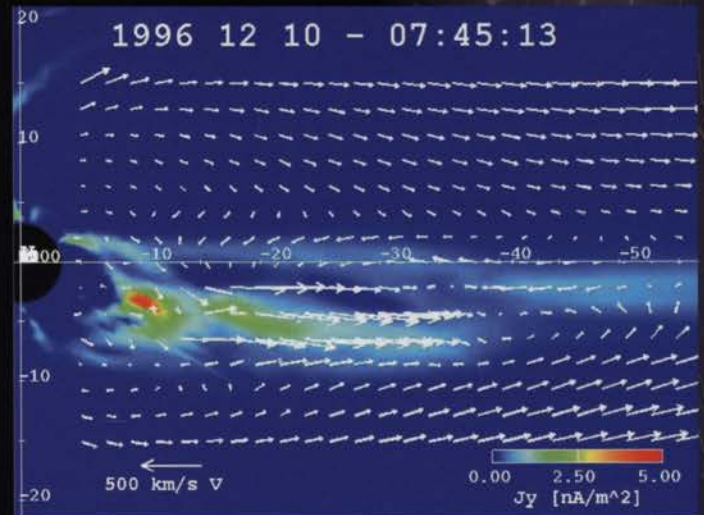
### Whims of the solar wind

A continuous flow of ionized hydrogen and helium—the plasma of solar wind—blows through space at about the speed of sound, carrying the sun's magnetic field with it. This field varies randomly, unlike the earth's field, in which magnetic field lines connect the north and south poles in a simple dipole. If plasma with an opposite flow hits the magnetosphere and is powerful enough, it seriously disrupts the magnetosphere. Some of the earth's field lines break, causing a substorm.

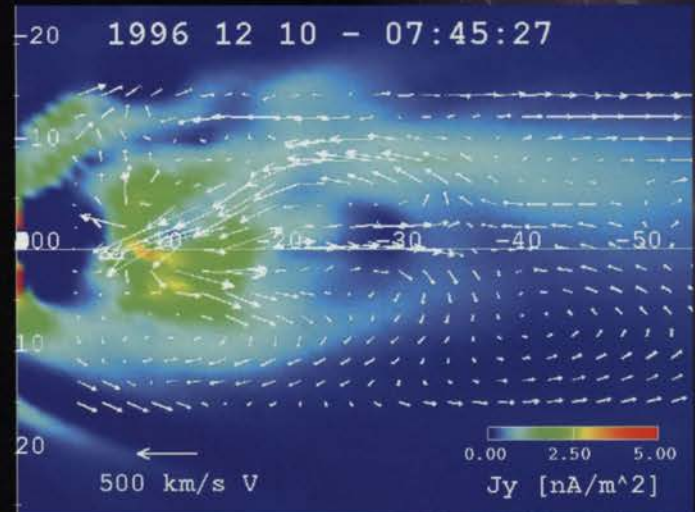
A magnetospheric substorm has three distinct phases: growth, expansion, and recovery. In the growth phase, the solar wind introduces stress into the system. During this phase, the earth's broken field lines merge with the sun's magnetic field carried by the solar wind. These "open field lines" are, in effect, the snagged ends of magnetic field lines from one of the earth's poles that connect instead to one of the sun's poles. Through them, energy and momentum transfer from the solar wind into the tadpole-shaped magnetosphere.

"As the stress increases, the system has to do something. What you get is an explosive release of energy and a magnetospheric substorm," says Wiltberger, an assistant research professor of physics and astronomy at Dartmouth. This release marks the beginning of the expansion phase, in which the open field lines reconnect to their appropriate poles on the earth. After the release of energy, the system slowly returns to normal during the recovery phase.

"One of the canonical questions in the study of magnetospheric storms is whether reconnection is the cause or the consequence of substorm onset," he says.



High-resolution substorm visualization showing reconnection flows propagating outward from the earth.



High-resolution substorm visualization.



## Connecting with reconnection

The answer to the chicken-or-the-egg puzzle of when reconnection occurs largely remains a mystery. As in previous studies, this international research team has seen large energy dissipation at substorm onset, as well as smaller, localized dissipation over time throughout the magnetosphere. Yet, because it is difficult to identify unique reconnection sites in computer simulations, no one has been able to tie reconnection events to these dissipations.

"Modeling the reconnection process in 3D is complex. But we do know that it doesn't resemble what is seen in traditional 2D models. Determining detailed boundary conditions for the location and intensity of reconnection sites would require a whole host of additional simulation runs," says Wiltberger. The team has been able to simulate the size, relative strength, and location of active reconnection regions, though, offering 3D simulations to track the density, heat, flow, and magnetic field direction of substorm plasma.

The simulations require about 12 hours to simulate six hours of magnetospheric activity on 16 processors of the Origin2000. The 3D magnetohydrodynamics code used by the team is an adaptation of a vector code with parallel directives written into the software, and it does not scale well beyond 32 processors. Beta testing is underway of a highly scalable version of the code that relies on the common message passing interface. This new code will allow the team to take advantage of newer systems like the commodity-based Linux terascale clusters at NCSA.

But the code is already helping to settle an ongoing debate in the study of magnetospheric substorms. Currently there are two schools of thought on where, not when, reconnection takes place. In the near-earth neutral line theory, reconnection starts about 30 earth radii out into the tail of the magnetosphere. In the competing current disruption theory, reconnection starts only about eight earth radii behind the planet and propagates away from the planet. Though there was some instability in the eight earth radii region, the research team saw that reconnection regions in their Origin2000 simulations never came much closer than 20 earth radii into the tail and that the reconnection process propagated away from the earth from there.

Verifying those results, however, will require more simulation runs. "Models of just a few events do not a theory make," as Wiltberger says.

## Should we talk about the weather?

Though the simulation results are tools in themselves for understanding the nature of the magnetosphere and its substorms, they are also part of the larger National Space Weather Project of the National Oceanic and Atmospheric Administration (NOAA), the Department of Defense, NASA, and the National Science Foundation. One of the space weather project's primary goals is to predict magnetospheric storms.

These bigger, less frequent disruptions to the magnetosphere can wreak havoc on communications systems and can black out power grids. A half-century ago, for example, current from a particularly nasty magnetospheric storm not only entered and interfered with telegraph systems but even melted telegraph keys at the ends of some lines, according to the Space Environment Center operated by NOAA and the U.S. Air Force. More recently—in 1989—a storm-induced blackout left about eight million Canadians without power. Today the outage of a single commercial satellite costs about \$1,000 per minute in lost revenue.

To forecast magnetospheric storms and other space weather in the vicinity of the earth, researchers need to model the behavior of other systems that cause and are influenced by magnetospheric storms. Magnetospheric substorms, which occur independently as well as during magnetospheric storms, are just one piece of this puzzle. Space weather prediction also requires good models of things like the solar wind and the earth's upper atmosphere. Without an all-inclusive model in which subsystems work together seamlessly, no one will be able to forecast when a storm might start, how it might progress, and what impact it might have.

So right now, the goals of the team using NCSA's Origin2000 are twofold: perfect the substorm model itself and begin folding it into a larger, comprehensive sun-magnetosphere-ionosphere model.

"We need to fully understand the fundamental magnetospheric response during storms and substorms," Wiltberger says. "But even when that is perfected, the larger, coupled space weather system will be crucial. Without an overall modeling system, we would have a leadtime of about 45 minutes. It would be like seeing the dark cloud overhead and predicting rain."

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**Access online** <http://access.ncsa.uiuc.edu/CoverStories/substorms/>

### For further information:

<http://myst.dartmouth.edu/wiltbemj/>

<http://www.sec.noaa.gov/>

### Team members

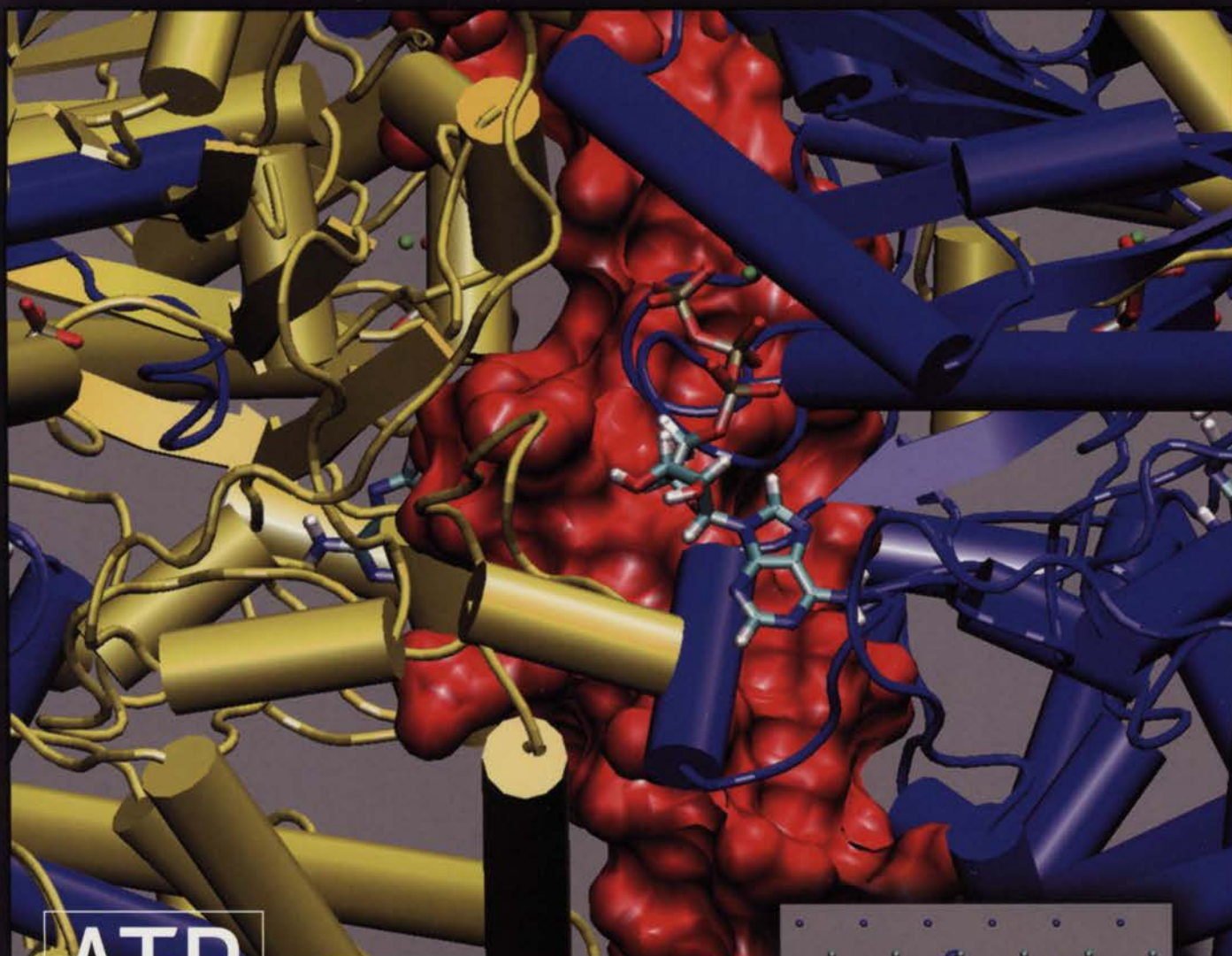
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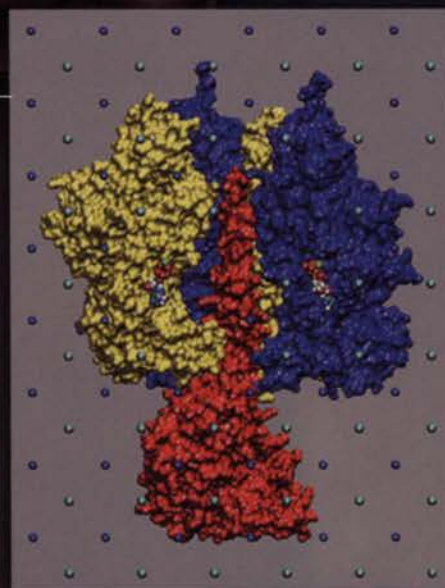


# ATP

ATP is the principal energy carrier in living cells. It is often synthesized from ADP and inorganic phosphate using a transmembrane proton gradient that is maintained by food molecule oxidation in animals or photosynthesis in plants and some bacteria. Energy released by the hydrolysis of ATP drives a number of vital biochemical reactions, including enzymatic catalysis and mechanical movements.

These visualizations of an ATP molecule in its binding site highlight two subunits of the F1 unit of an enzyme known as F<sub>0</sub>-F<sub>1</sub> ATP-synthase. The alpha subunit is shown in yellow, the beta subunit in blue. (The inset image shows the whole enzyme, the large image zooms in on the binding site.) The enzyme uses the mechanical force generated by the rotation of its transmembrane unit, F<sub>0</sub>, to catalyze ATP synthesis in the catalytic F<sub>1</sub> unit. These units interact mechanically through the central stalk, shown in red.

A full atomic-level model of the F<sub>1</sub> unit in an aqueous environment was recently created by Barry Isralewitz, Klaus Schulten, and Emad Tajkhorshid of the Theoretical Biophysics Group at the University of Illinois. The simulation included 327,000 atoms, captured one nanosecond of the unit's molecular dynamics, and required 10 days of computing time on the Alliance's 256-processor Origin2000 supercomputer at NCSA.





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